

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.31e-04 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.98e-01

Confidence level: 4.06e-01

Nearest Neighbors from the Training Set

Image not found

Cyclobutane, octafluoro-

Measured: 1.65e-04

Predicted: 1.51e-04

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Ethane, hexafluoro-

Measured: 5.64e-05

Predicted: 1.08e-04

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Carbon tetrafluoride

Measured: 2.14e-04

Predicted: 2.75e-04

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Bromotrifluoromethane

Measured: 2.15e-03

Predicted: 2.18e-03

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1,2-Dibromo-1,1,2,2-tetrafluoroethane

Measured: 1.15e-05

Predicted: 4.98e-05